Atomic and Molecular Spectroscopy

Course Code: PHYS4009

LECTURE TOPIC

X-Ray Spectroscopy

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Please see the vedio lecture at
https://www.youtube.com/watch?v=nzApSKIx3b0

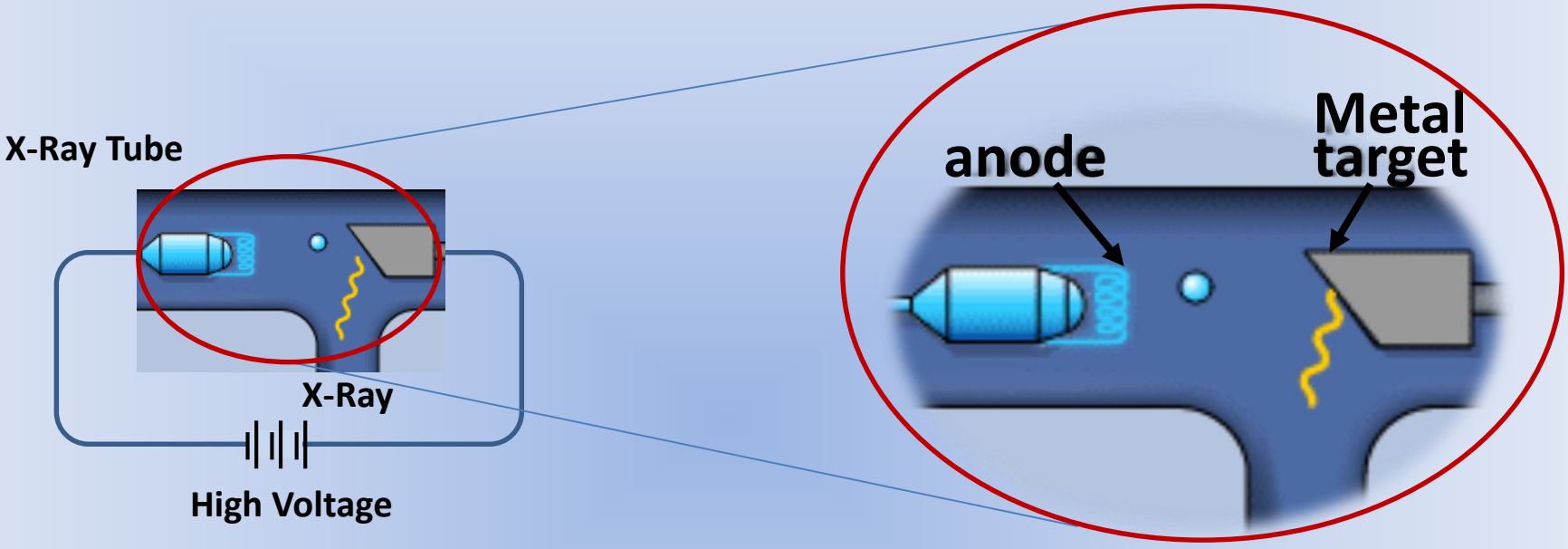
Introduction

X-rays were discovered by the German physicist W. C. Röntgen in 1895.

Röntgen accidentally noticed that fluorescent materials showed a faint glow when placed near a cathode-ray tube powered by a high voltage induction coil.

Since he was the first one who observed "a new kind of rays". He called them "X-rays" (X=unknown). Thereafter, he started systematic research on their properties.

Production of X-Ray



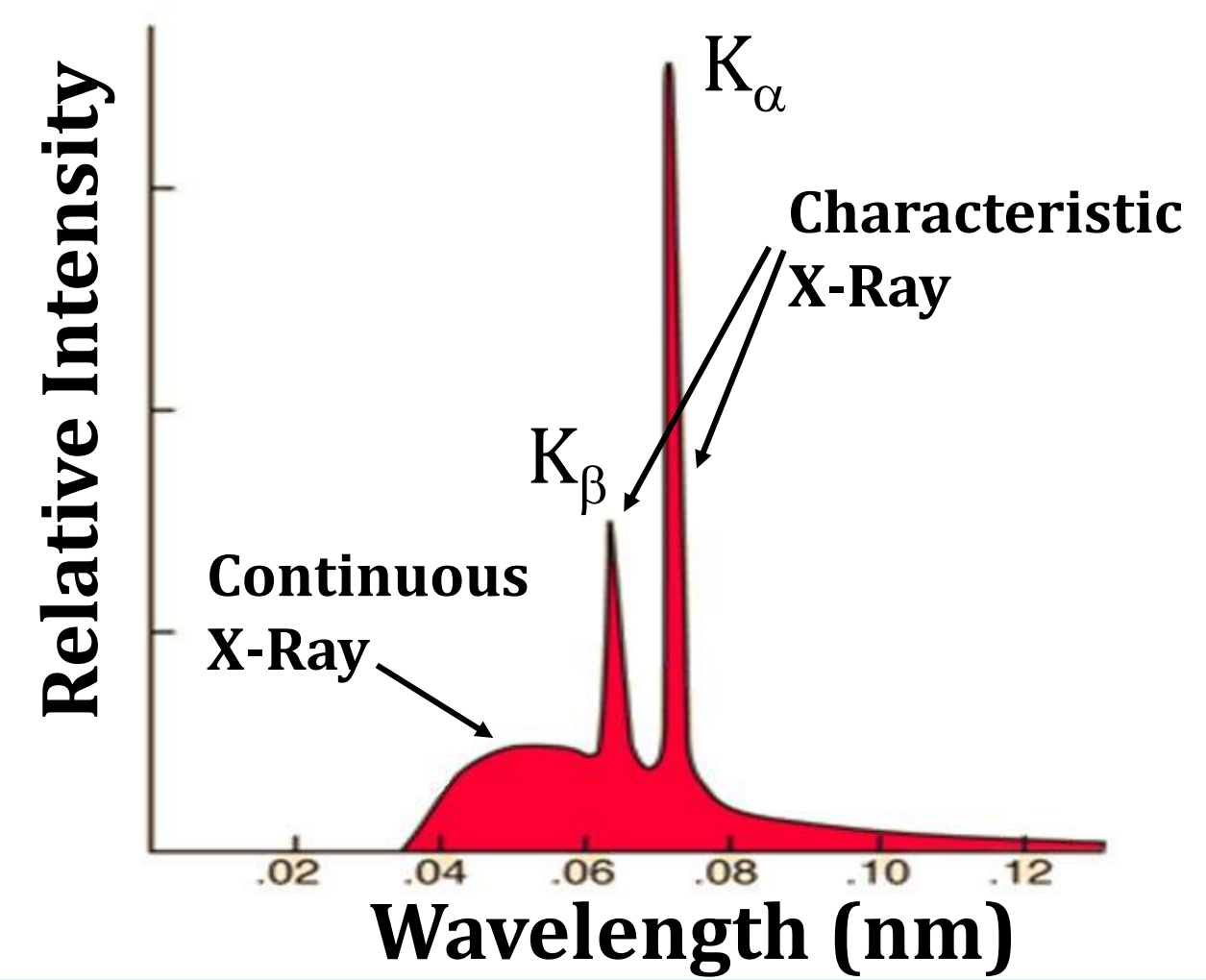
X-rays are produced by accelerating electrons with a high voltage and allowing them to collide with a metal target.

Properties of X-Rays

- X-rays are invisible electromagnetic radiation having wavelength ranging from 0.01 nm to 10 nm which are shorter than those of UV rays and typically longer than those of gamma rays.
- Unaffected by electric and magnetic fields.
- Capable of ionizing gases.
- Capable of inducing biological reactions.

X-Ray Spectrum

X-ray spectrum is represented by a **graph** showing the relative intensity of **x-rays** emitted by a source at different wavelengths.



Characteristic X-Ray

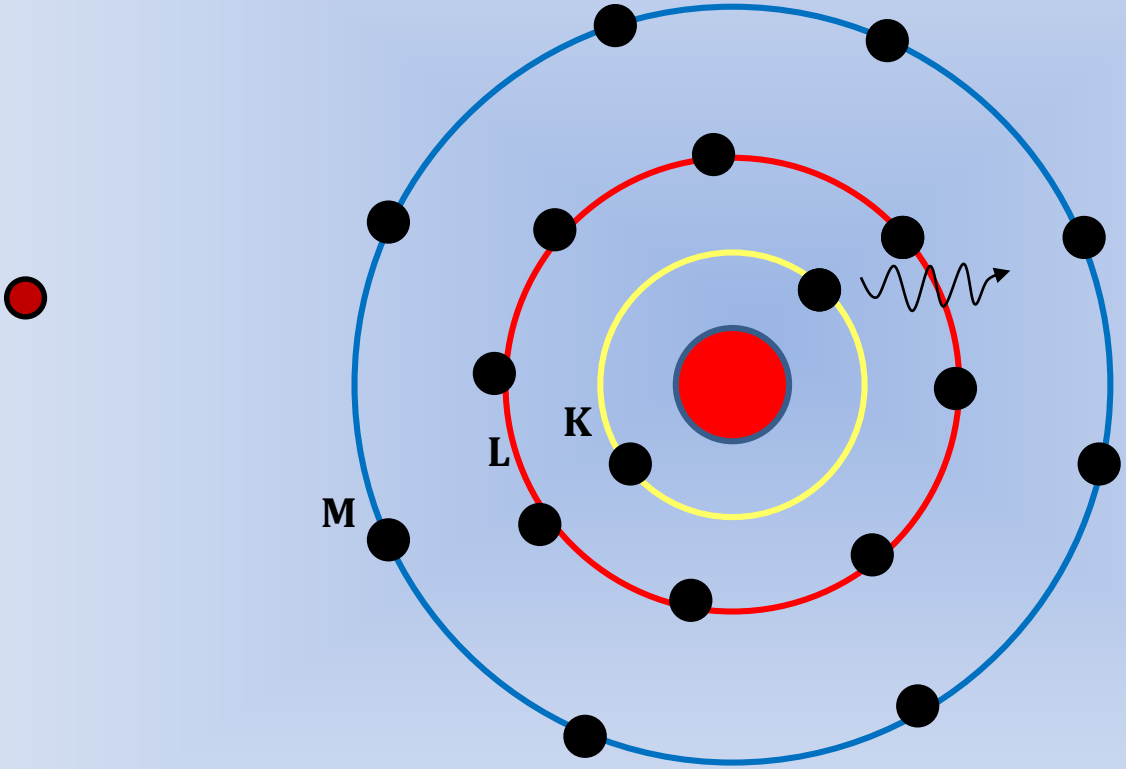
Characteristic x-rays are emitted when high energy electron hits the target of heavy element.

The bombarding electrons ejects electrons from the inner shells of the atoms of the metal target and creates a vacancy. These vacancies are quickly filled by electrons from higher energy levels, emitting x-rays with sharply defined frequencies associated with the difference between the atomic energy levels of the target atoms.

The characteristic x-ray emission are the two sharp peaks in the X-Ray spectrum.

Origin of Characteristic X-Ray

Bombarded Electron



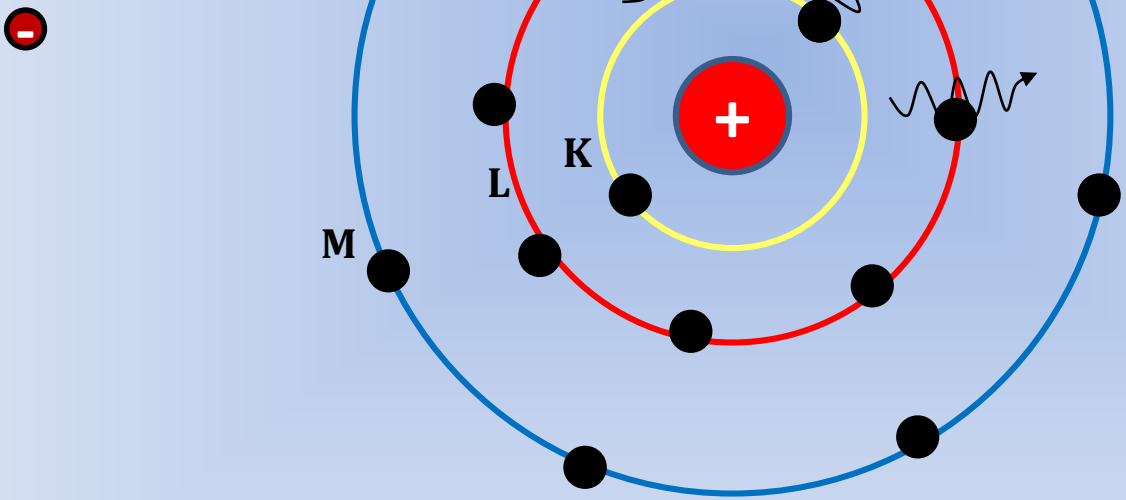
K_α

Core Electron

The energy absorbed by an atom get transfer's to the electrons of inner core shells of the atom which are then ejected from the atom and vacancy is created. The atom is left in an excited state with an empty electronic level. The vacancies quickly gets filled by dropping down the electrons from higher energy levels, emitting the x-rays with sharply defined frequencies associated with the difference between the atomic energy levels of the target atoms. Any excess energy is given to the ejected photoelectron.

The x-rays produced by transitions from L to K level are called K_α x-rays, and those starting from M to K level transition are called K_β x-rays.

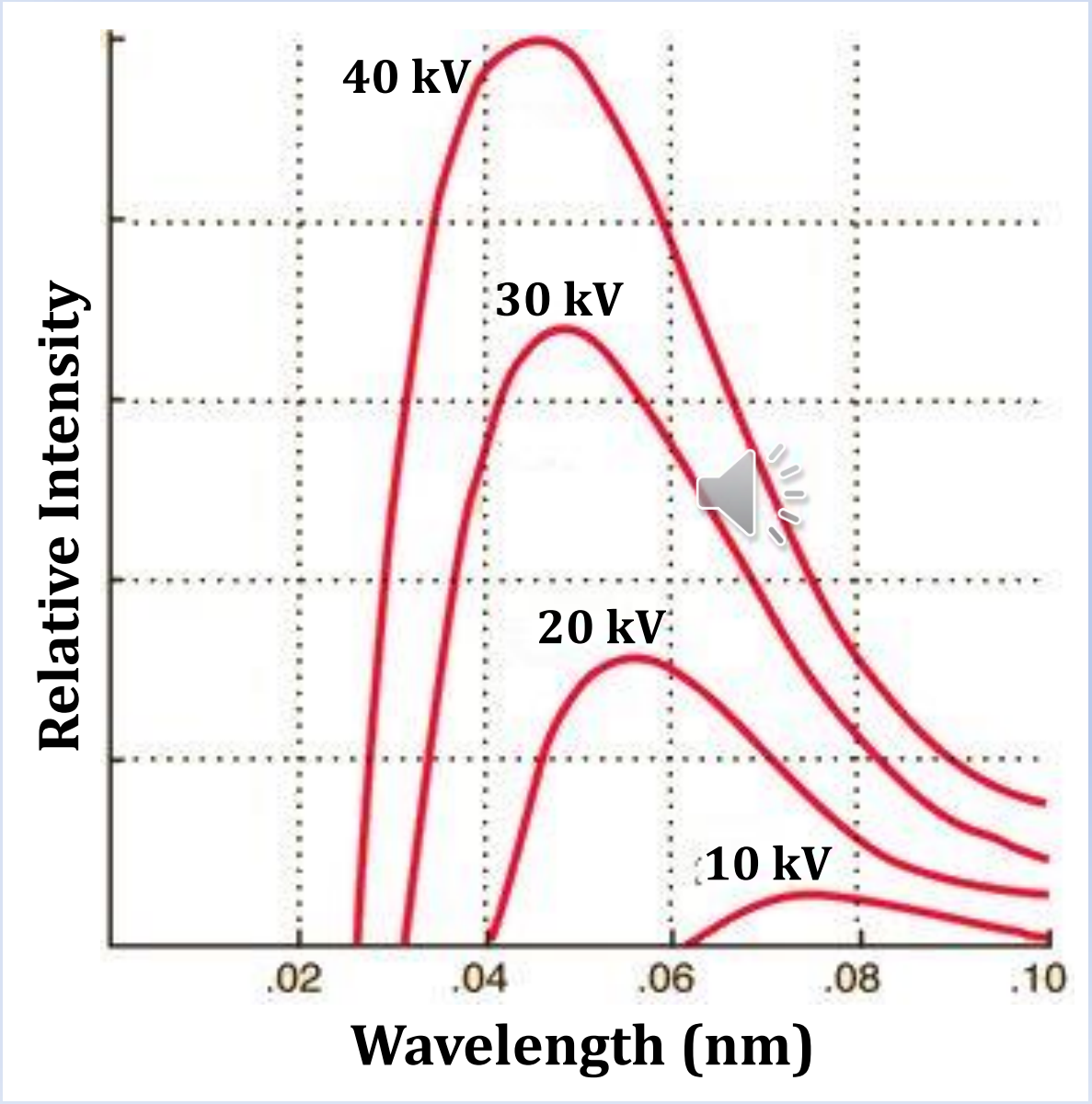
Origin of Continuous X-Ray



Accelerated electrons emits radiation "**Bremsstrahlung**"

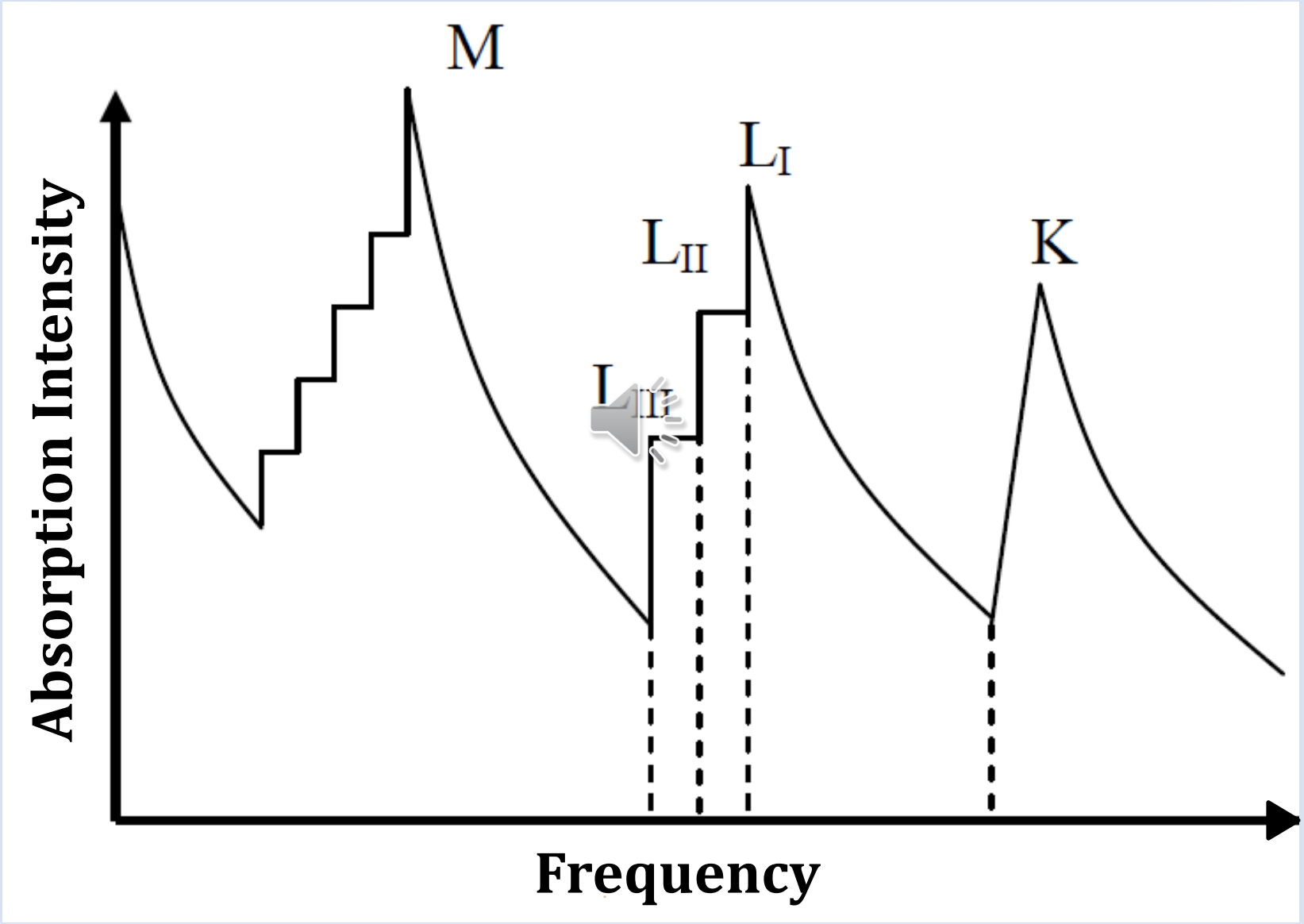
"Bremsstrahlung" is a German word which means "**braking radiation**". It is emitted when electrons are decelerated or "braked" while passing by the positive charged nucleus of the atoms of the target. Accelerated charges give off electromagnetic radiation, and when the energy of the bombarding electrons is high enough, that radiation is in the x-ray region of the electromagnetic spectrum. It is characterized by a continuous distribution of radiation. It becomes more intense and shifts toward lower wavelength when the energy of the bombarding electrons is increased.

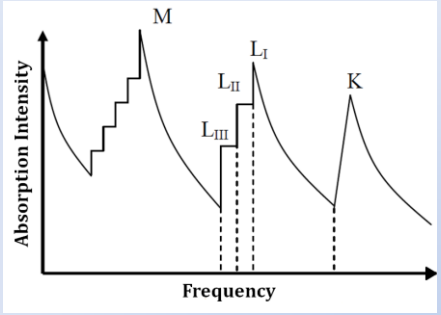
Peak shifts towards lower wavelength



Become more intense at lower wavelength

Absorption Spectrum of X-Rays





The spectrum show sharp discontinuity in the absorption spectrum of a substance.

These discontinuities occur at frequencies where the energy of an absorbed photon corresponds to an electronic transition or ionization potential. When the energy of the incident radiation becomes smaller than the work required to eject an electron from one or other energy states in the constituent absorbing atom, the incident radiation ceases to be absorbed by that state. For example, incident radiation on an atom of a frequency that has a corresponding energy just below the binding energy of the K-shell electron in that atom cannot eject the K-shell electron. Similarly, for the case of L and M-shell electrons.

We have observed that the X-ray spectra show set of discrete lines. They are designated as K-series, L-series, M-series, etc.

The first line of K-series is K_α. The wavenumber corresponding to the K_α line for the atoms with different atomic number Z can be expressed as:

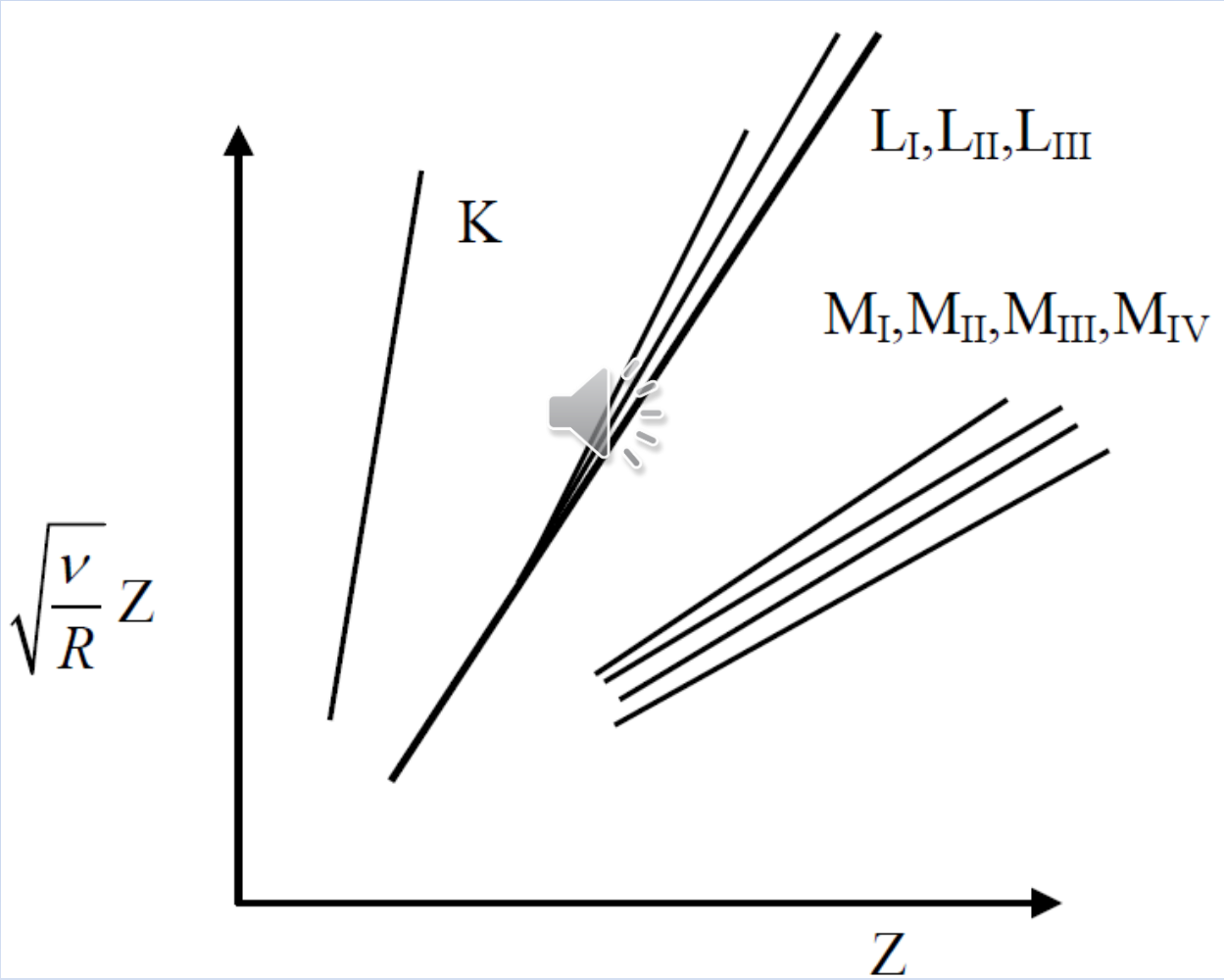
$$\bar{\nu}_{K\alpha} = R(Z - \sigma_k)\left(\frac{1}{1^2} - \frac{1}{2^2}\right)$$

Similarly, the expression for the first line of L-series i.e. L_α is:

$$\bar{\nu}_{L\alpha} = R(Z - \sigma_l)\left(\frac{1}{2^2} - \frac{1}{3^2}\right)$$

where, R = Rydberg Constant and σ_k and σ_l represent the screening constant for the lines for K-series and L-series, respectively.

If we plot the $\sqrt{\nu}$ vs Z graph for different elements, we observe linear relationship. This is known as Moseley's law.



Moseley's diagram of X-ray absorption edges

Screening Doublet Law

As we see that X-ray spectra has certain doublets for which the Moseley plots show parallel lines. These doublets are called "screening doublets" as it arise essentially due to the difference in screening.

For pair of line the difference $\sqrt{\nu/R}$ is a constant and essentially independent to Z which is the characteristic of screening doublet is known as "screening doublet law".

The two levels with same n and l but different directions of spin, that is, with different values of j are called spin doublet.

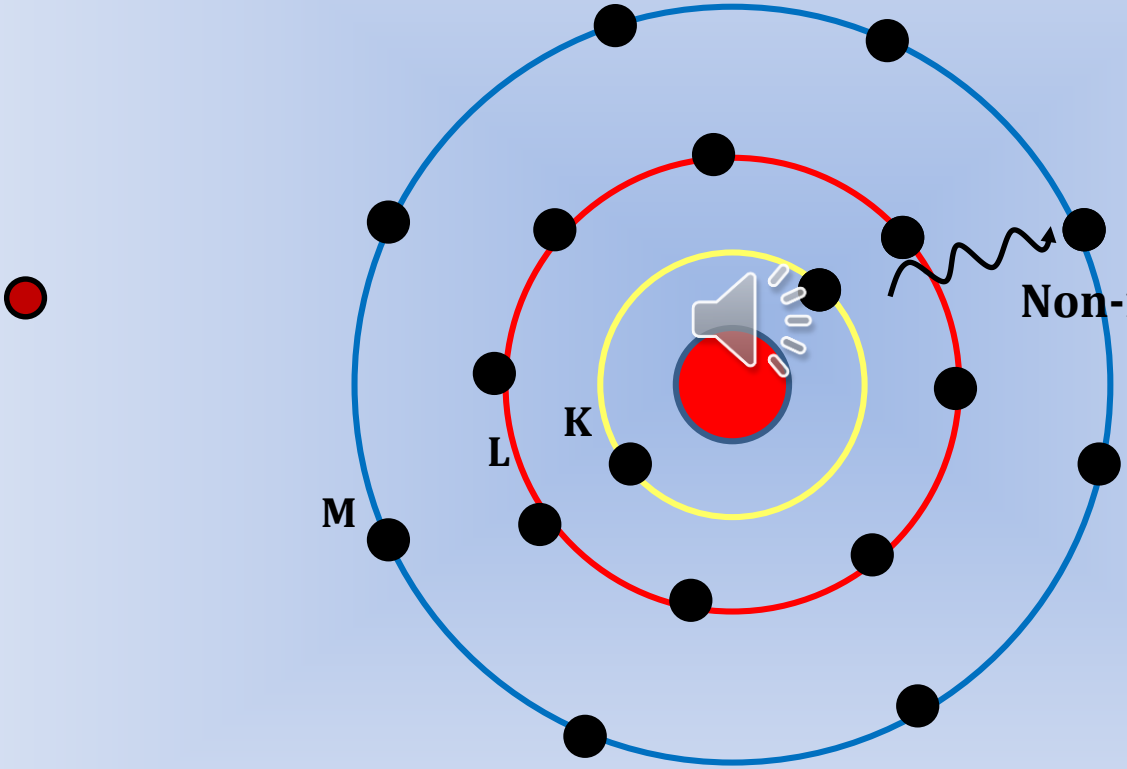
The energy difference between two spin-relativity doublet is proportional to the fourth power of $(Z - \sigma)$, where σ (n,l) is the internal screening constant which is appropriate for the spin-orbit interaction. This is called spin-relativity doublet law.

Auger Effect

The Auger effect is a physical phenomenon or process by which electrons with characteristic energies are ejected from the outer energy level of the atoms in response to the filling of an inner-shell vacancy of an atom by another electron in the atom.

In this process when an inner shell electron is removed from an atom, an electron from a higher level quickly make the transition downward to fill the vacancy. Sometimes this transition is accompanied by non-radiative energy. The energy released by the downward transition is given to one of the outer electrons instead of emitting a photon, and this electron is then ejected from the atom with an energy equal to the energy lost by the electron which made the downward transition minus the binding energy of the electron that is ejected from the atom.

Auger Process



What we learned?

- **What are X-rays and how they are produced?**
- **Properties of X-rays.**
- **Types of X-rays and its origin**
- **X-ray absorption and its characteristic properties**
- **Moseley's Law**
- **Screening effect on X-ray spectra**
- **Auger Effect**

Suggested Books for Reading

1. Atomic & Molecular Spectra by Raj Kumar
2. X-Ray Spectroscopy. An Introduction. By B. K. Agarwal

Thank You